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Citation for the original published paper (version of record):

Michelsen, J., Shumeiko, V. (2009). Quantum phase dynamics of high-T_c Josephson junctions. *Journal of Physics: Conference Series*, 150: 052159-.
<http://dx.doi.org/10.1088/1742-6596/150/5/052159>

N.B. When citing this work, cite the original published paper.

Quantum Phase Dynamics of High- T_c Josephson Junctions

Jens Michelsen and Vitaly Shumeiko

Chalmers University of Technology, SE-41296 Göteborg, Sweden

E-mail: jens.michelsen@mc2.chalmers.se

Abstract. We study quantum phase fluctuations in planar junctions between high- T_c superconductors for a range of relative orientations of the a-b crystal axes. Specifically, attention is directed towards the fermionic subspace of low energy Andreev bound states, midgap states (MGS). This subspace, being responsible for most of the Josephson current, strongly couples to the phase degree of freedom. Low frequency phase fluctuations may introduce intrinsic dynamics in this subspace, which would lead to a strong dynamical modulation of the Josephson current, and thus affect the phase quantum dynamics. In this article it is found that transitions between pairs of MGS induced by the phase fluctuations are forbidden due to specific symmetry properties of the MGS, and the macroscopic quantum Hamiltonian remains essentially adiabatic within the assumption of a specular interface.

Introduction. Recent experiments demonstrated that superconducting circuits containing Josephson tunnel junctions exhibit coherent macroscopic quantum dynamics, and may serve as building blocks of quantum processors [1, 2]. Macroscopic quantum tunneling has also been observed in junctions of high- T_c superconductors [3, 4], and potential qubit applications have been theoretically discussed [5, 6]. The quantum mechanical variables in these systems are the differences in superconducting phases across the junctions, while the conjugated variables are the charges accumulated on the junction capacitors. Due to a large energy gap in the quasiparticle spectrum of Josephson tunnel junctions of low- T_c s-wave superconductors, the quasiparticle transitions induced by low frequency phase fluctuations are exponentially weak at small temperature, $\omega, T \ll \Delta$, and therefore the dissipation effect is negligible [7, 8, 9, 10]. This is the fundamental reason why macroscopic quantum coherence exists.

The situation in high- T_c superconductors is different. Due to the d-wave symmetry of the order parameter, there are low energy, nodal fermionic excitations, whose non-adiabatic dynamics affects the quantum dynamics of the phase fluctuations. This problem has attracted considerable attention, and dissipation due to the nodal quasiparticles has been investigated [12, 13, 14, 15, 16]. At small frequencies, the nodal quasiparticles that efficiently interact with phase fluctuations occupy a small phase volume, roughly proportional to the ratio ω/Δ_0 , where Δ_0 is the maximum gap value, and therefore the effect on the macroscopic quantum dynamics is relatively small. This conclusion concerns both the continuum nodal states and the Andreev bound states situating close to the gap edges.

Potentially more significant effect on the macroscopic quantum coherence might be expected from the midgap states (MGS), the Andreev bound states situating close to the Fermi surface [19, 20]. MGS are formed wherever quasiclassical electronic trajectories connect order parameter lobes of different signs. The phase volume occupied by the MGS depends on the junction

geometry, and generally it is not small, except of particular junction orientations. Therefore the effect of the MGS can be much larger than that of the nodal states. Moreover, since MGS carry a considerable fraction of the Josephson current, they can produce not only dissipation, but also affect the dynamic part of the macroscopic quantum Hamiltonian.

In this article we investigate the MGS dynamics under time variation of the superconducting phase difference. We find that MGS are protected against the interlevel transitions due to specific symmetry of the MGS wave functions. Thus the MGS response is essentially adiabatic: it contains no dissipation, and it contributes to the quasistatic Josephson potential in the macroscopic quantum Hamiltonian as was assumed in [14, 15, 17].

Effective action. To investigate the dynamics of the MGS we use a modified path integral method of references [7, 8, 9, 10, 11], where the exact contact eigenfunctions are used instead of the tunnel Hamiltonian, and consider the action of the contact,

$$S[\varphi, \bar{\psi}, \psi] = \int_{\mathcal{C}} dt \left(\frac{1}{4E_c} \dot{\varphi}^2 - V_{\text{ext}}(\varphi) \right) + S_{\text{qp}}[\varphi, \bar{\psi}, \psi]. \quad (1)$$

Here the first two terms are due to the coupling of the phase variable to the electromagnetic gauge fields; $E_c = (2e)^2/2C$ is the junction charging energy, $V_{\text{ext}}(\varphi)$ refers to the inductive energy either of the SQUID loop or the bias current; the integration is taken along the Keldysh contour \mathcal{C} . Throughout this article we shall use units where $\hbar = c = 1$.

The last term in Eq. (1), S_{qp} , describes the coupling of the phase variable to the fermionic quasiparticles:

$$S_{\text{qp}}[\varphi, \bar{\psi}, \psi] = \int_{\mathcal{C}} dt \left(\bar{\psi} \left[i\partial_t - \hat{H}(\varphi) \right] \psi \right), \quad (2)$$

where H denotes the full single-particle mean-field Hamiltonian, including the interface potential. It is written in Nambu-form, $\psi = (\psi_{\uparrow}, \psi_{\downarrow}^{\dagger})^T$ and depends parametrically on time through $\varphi(t)$. We expand the fields, $\psi(\vec{r}, t) = \sum_i \phi_i(\vec{r}) a_i(t)$, using an instantaneous eigenbasis $\{\phi_i(\vec{r})\}_{\varphi(t)}$. The expansion coefficients a_i are Grassmann variables, in terms of which the action takes the form:

$$S_{\text{qp}}[\varphi] = \sum_{ij} \int_{\mathcal{C}} dt \bar{a}_i(t) [i\partial_t \delta_{ij} - E_{ij}(\varphi) + \dot{\varphi} A_{ij}(\varphi)] a_j(t). \quad (3)$$

Here the diagonal matrix $E_{ij}(\varphi) = \langle \phi_i | H(\varphi) | \phi_i \rangle \delta_{ij}$ corresponds to the instantaneous eigenenergies, and

$$A_{ij}(\varphi) = i \langle \phi_i | \partial_{\varphi} \phi_j \rangle = \frac{\langle \phi_i | i \partial_{\varphi} H | \phi_j \rangle}{E_i - E_j} \quad i \neq j, \quad (4)$$

describes transitions between the states due to time-dependence of the phase. Since we will be concerned with the dynamics of the Andreev bound states, we truncate the description to this subspace by reducing the sum in Eq. (3) to the bound states.

To obtain the matrices \mathbf{E} and \mathbf{A} one should evaluate the spectrum and wave functions of the bound states for a given junction geometry. The single particle Hamiltonian of our problem has the form,

$$\hat{H}(\varphi) = (\hat{\epsilon} + \hat{U})\sigma_z + \hat{\Delta} [\cos \varphi \sigma_x + \text{sign}(x) \sin \varphi \sigma_y], \quad (5)$$

where \hat{U} represents the interface potential centered at $x = 0$ and extended on a distance much smaller than the superconducting coherence length (short junction). The kinetic energy, and the order parameter are represented by $\hat{\epsilon}$ and $\hat{\Delta}$, respectively. In this paper we shall assume specular reflection and neglect, within the quasi-classical approximation, the overlap between the states of different trajectories. The general properties of the Andreev bound states of this Hamiltonian are as follows [18, 20, 21]: For each quasi-classical trajectory there exist at most two bound states. Such states belong to one of two types, depending on the particular orientations of the

crystal axes of the junction electrodes: edge gap states (EGS), or midgap states (MGS). The EGS are formed at the trajectories that connect order parameter lobes with the same sign, in tunnel junctions they situate close to the gap edges; MGS exist at trajectories connecting the lobes with different signs, and have energies close to the Fermi level [19].

Selection rule. In order to proceed let us look at typical orientations of the crystal axes for which both MGS and EGS exist, namely the symmetric orientation where the crystal \hat{a} axis of both superconductors is rotated by an angle θ relative to the \hat{x} axis, see Fig. 1. The order parameter for a given momentum $\vec{k}_F = k_F(\sin \vartheta, \cos \vartheta)$ is then given by $\Delta(\vartheta) = \Delta_0 \cos(2(\vartheta - \theta))$. The reflected momentum will have a corresponding angle $\pi - \vartheta$. The MGS spectral equation for a given trajectory reads,

$$\cos^2 \left(\frac{\eta^+ + \eta^-}{2} \right) = D \cos^2 \left(\frac{\eta^+ - \eta^- + \varphi}{2} \right), \quad (6)$$

where $\eta^\pm = \arccos(E/|\Delta^\pm|)$. $\Delta^\pm(\vartheta) = \Delta_0 \cos(2(\vartheta \mp \theta))$ denotes the order parameter for trajectories going in the positive/negative x -direction, and $D(\vartheta)$ is the angle dependent transparency of the junction. This spectral equation possesses the symmetry: if E_1 is a solution, then so is E_2 , $\eta^\pm(E_2) = \pi - \eta^\mp(E_1)$.

Furthermore the junction geometry is symmetric under combined charge conjugation ($C : H \rightarrow H^*$) and parity inversion ($P_{\vec{r}} : \vec{r} \rightarrow -\vec{r}$). The wave functions of the bound states then satisfy $CP\phi_s(\vec{r}) = \phi_s^*(-\vec{r}) = \lambda_s \phi_s(\vec{r})$, where $\lambda_s \in \{1, -1\}$ is the eigenvalue under the symmetry transformation.

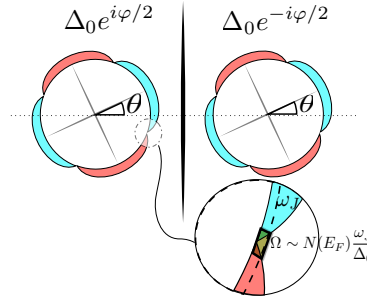


Figure 1. Symmetric orientation of the crystal axes. The symmetry with respect to charge conjugation $\varphi \rightarrow -\varphi$ combined with parity inversion $\vec{r} \rightarrow -\vec{r}$ is obvious. The inset shows the phase-space volume of EGS for which transitions may be induced.

The expression for λ_s for a given trajectory can be obtained from the matching condition at the contact. Using a general unitary- and time reversal invariant scattering matrix to describe the interface potential, and matching elementary solutions of the Hamiltonian of the bulk electrodes ($U=0$), we obtain for the MGS the following expressions for lambda:

$$\lambda_s = \frac{1}{\sqrt{D}} \frac{\cos \left(\frac{\eta^+(E_s) + \eta^-(E_s)}{2} \right)}{\cos \left(\frac{\eta^+(E_s) - \eta^-(E_s) + \varphi}{2} \right)}. \quad (7)$$

Using the relationship $\eta^\pm(E_2) = \pi - \eta^\mp(E_1)$ one can now easily establish that $\lambda_2 = -\lambda_1$. Since the operator $\partial_\varphi H$, the matrix elements of which provide expressions for A_{ij} according to Eq.(4), is also invariant under this transformation, transitions will not be allowed between states that belong to different submodules of the symmetry operator. From this analysis it follows that for the MGS the matrix elements $A_{ij} = 0, i \neq j$.

Using similar arguments this result can be shown to hold also for antisymmetric junctions. Deeper analysis suggests that the selection rule is closely related to the level crossing of MGS at

various $\varphi = n\pi$. The crossing persist for all misorientation angles indicating that the selection rule is a general property of MGS.

A similar analysis performed for the EGS shows that $\lambda_2 = \lambda_1$, and therefore the transitions are allowed. However, the contribution of these states is small. Indeed, the transitions between the EGS can only be induced if the frequency ω of the phase fluctuations is comparable to the local superconducting gap $\omega \sim \Delta(\vartheta) \approx \vartheta\Delta_0$. Therefore the effective trajectories are in the nodal region within the range $\delta\vartheta \sim \omega/\Delta_0$, and their contribution to the macroscopic quantum Hamiltonian is small.

Neglecting the effect of the nodal EGS, we evaluate the contribution of the bound states to the macroscopic quantum Hamiltonian in the adiabatic approximation. To this end we perform a partial trace over the bound state variables a_i, a_i^\dagger in truncated Eq. (3), $iS_{\text{qp}} = \text{Tr} \ln[-i\mathbf{G}_0^{-1}]$, where $\mathbf{G}_0^{-1} = (i\partial_t - \mathbf{E})$ and \mathbf{E} is a diagonal matrix containing MGS and EGS energies. Using a method similar to the one introduced in reference [11], this can be written in an explicit form,

$$\text{Tr} \ln[-i\mathbf{G}_0^{-1}] = -i \int_C dt \frac{1}{2e} \int d\varphi' I_J(\varphi') = -i \int_C dt V_J(\varphi), \quad (8)$$

where $I_J = 2e \sum_i (\partial E_i / \partial \varphi) n_i^0$ is the non-equilibrium Josephson current; n_i^0 is the Fermi distribution corresponding to an initially thermalized state at initial phase φ_0 , $n_i^0 = (e^{\beta E_i(\varphi_0)} + 1)^{-1}$. $V_J(\varphi)$ is the resulting Josephson potential entering the macroscopic quantum Hamiltonian.

Conclusion. We have demonstrated that the different types of low energy MGS are protected against transitions and thus provide a static Josephson potential even in the presence of low frequency phase fluctuations. EGS on the other hand are situated at the edges of the gap and transitions therefore will only be possible for trajectories very close to the gap nodes. The dominant contribution to the Josephson potential can therefore be treated adiabatically providing a justification for the static potential commonly used in several articles [14, 15, 17]. This work has been supported by Swedish Research Council (VR), Swedish Strategic Foundation, and EU-MIDAS consortium.

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